

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.14 days

Global applicability domain: Outside

Local applicability domain index: 7.45e-02

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylhexane</div> <div>Measured: 12.5</div> <div>Predicted: 5.54</div>	<div>Image not found</div> <div>2-Methylheptane</div> <div>Measured: 12.5</div> <div>Predicted: 3.99</div>	<div>Image not found</div> <div>3-Methylhexane</div> <div>Measured: 157</div> <div>Predicted: 6.83</div>
<div>Image not found</div> <div>2-Methyloctane</div> <div>Measured: 40.7</div> <div>Predicted: 4.23</div>		